Breaking the Rules: An Organic Molecule with an "Open-Shell Doublet" Ground State

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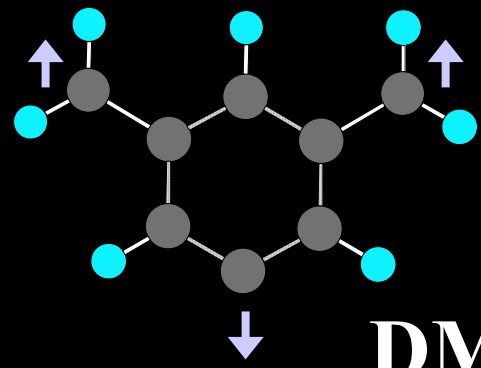
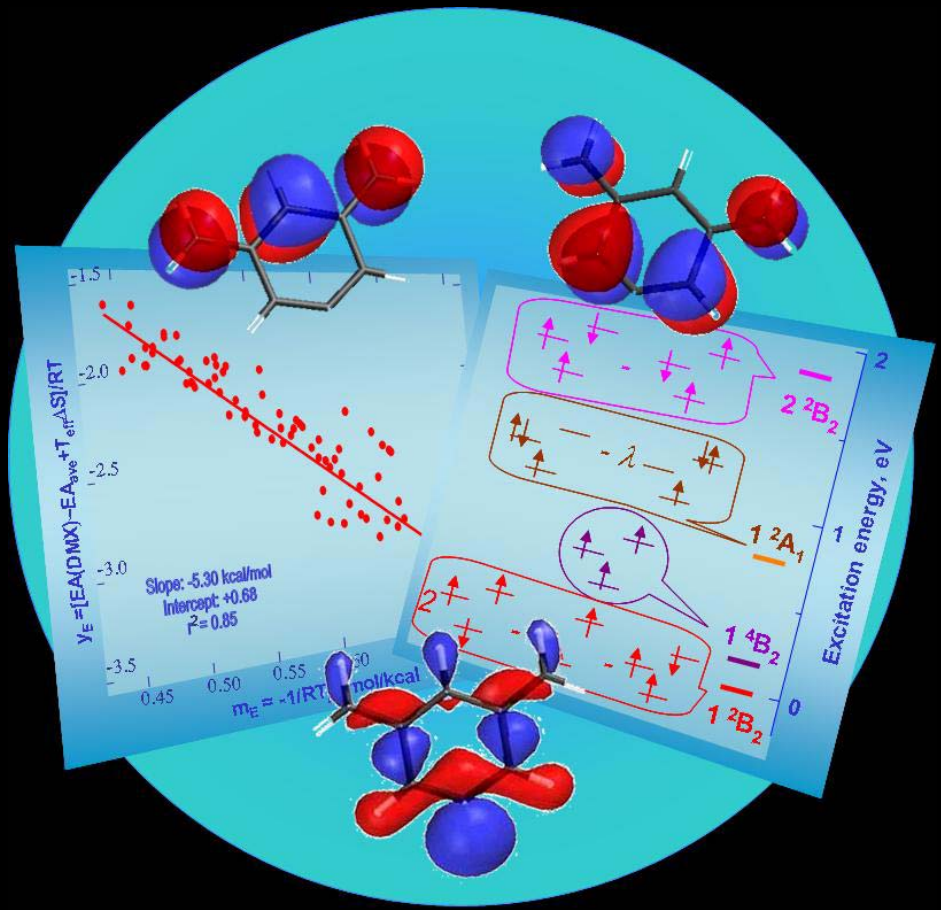


DMX



Experimental and theoretical studies carried out at Purdue University and the University of Southern California find that the 5-dehydro-*m*-xylylene (**DMX**) triradical has an "open-shell doublet" ground state, consisting of three unpaired electrons that are antiferromagnetically (low-spin) coupled. This electron arrangement is contrary to what is expected by Hund's Rule, and is unprecedented for a ground state hydrocarbon. The figure to the left shows the non-bonding molecular orbitals in the triradical and plots highlighting the complimentary results obtained from experiment and theory.

Slipchenko, L. V., Munsch, T. E., Wenthold, P. G., Krylov, A. I.
Angew. Chem., Int. Ed. Eng. **2004**, *43*, 742 - 745